

Spectroscopic Database Needs for UV/VIS Satellite Measurements of Atmospheric Trace Gases

K. Chance

Smithsonian Astrophysical Observatory

E. Hilsenrath

NASA Goddard Space Flight Center

**Workshop on Spectroscopic Needs
for Atmospheric Sensing**

San Diego, California

October 2001

Outline

- Overview of trace gas measurement needs
- UV/VIS radiances
- Satellite Instruments
- Status and needs in UV/VIS spectroscopic database

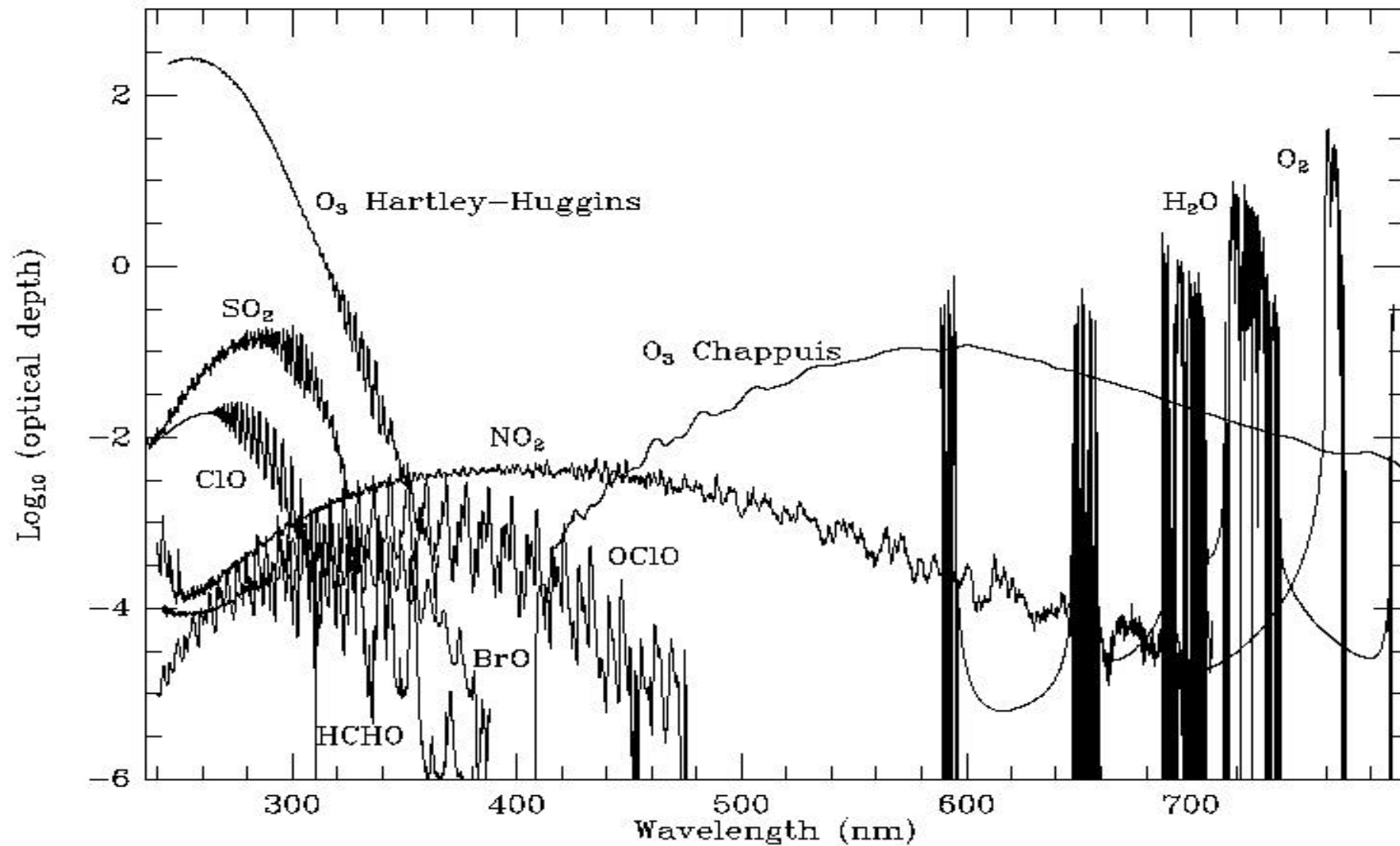
Remote Sensing in UV/VIS/NIR

- Measurements of ozone depletion, air quality, and climate can be measured by observing reflected radiation from the surface or scattered radiation from atmosphere.
- Measurements in NIR (700 nm to 2.5 microns)
 - CO_2 , CO , CH_4 , H_2O ; climate, air quality, and transport
 - O_2 A; cloud heights, s/c pointing, and temperature/pressure profiles with sufficient spectral resolutions.
- Constituents observable from 270 to ~650 nm are the subject of this talk.

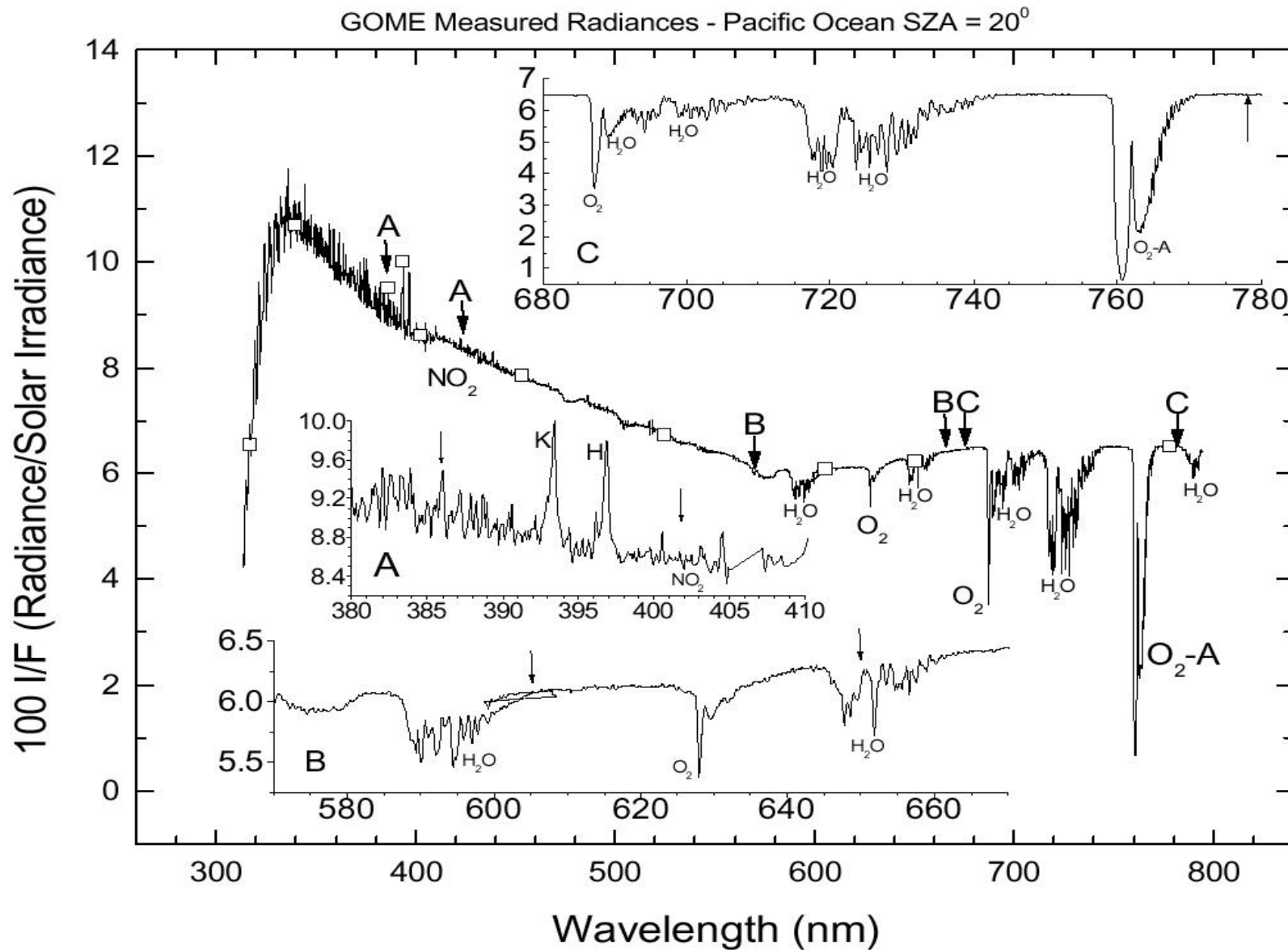
Reflected/Backscatter radiation retrievals

- For ozone, which is optically thick (UV), cross sections and instrument calibration are main sources of errors. Forward models are very accurate.
- For optically thin gases, spectral fitting of measured radiances, compared to cross sections yields slant column amounts.
 - *Slant column* amounts ~ absorption of solar photons from the top of the atmosphere back to space instrument.
 - Air mass factor needed to convert to *vertical column* amounts for nadir measurements.
 - Spectroscopic errors become less important compared to forward model and retrieval errors.
 - Interference from strong absorbers (ozone) and Ring effect (reflected Fraunhofer lines) must be accurately accounted for.
 - Instruments need high S/N (>2000) and very good wavelength calibration.

Gases Observable in UV/VIS/NIR



Radiances observed in UV/VIS/NIR



UV/VIS/NIR satellite spectrometers

Instrument	Wavelength (nm)	Viewing geometry	Gases†	Year
TOMS	300-380	nadir	O ₃ , Column	1978
SBUV/POESS	250-405	nadir	O ₃ , Column and profile	1978
POAM	350-1060	occultation	O ₃ , NO ₂ , H ₂ O	1993
GOME (GOME-2)	240-790	nadir	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO, H ₂ O	1995 (2005)
ODIN/OSIRIS	280-800	limb	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO, H ₂ O	2000
SAGE III	280-1040	occultation (limb)	O ₃ , NO ₂ , BrO, OCIO, H ₂ O, NO ₂	2001
GOMOS/Envisat	250-952	stellar occultation	O ₃ , NO ₂ , H ₂ O, NO ₃	2002
SCIAMACHY/Envisat		nadir/limb/occultation	O ₃ , H ₂ O, NO ₂ , NO ₃ , N ₂ O, CH ₄ , CO, CO ₂ , BrO,	2002
OMI/Aura	270-500	nadir	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO	2003
MAESTRO /ACE	285-1030	occultation	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO, H ₂ O	2003
ODUS/GCOM	306-420	nadir	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO	2006
OMPS/NPOESS	250-1000	nadir/limb	O ₃ , NO ₂ , BrO, OCIO, SO ₂ , HCHO	2010

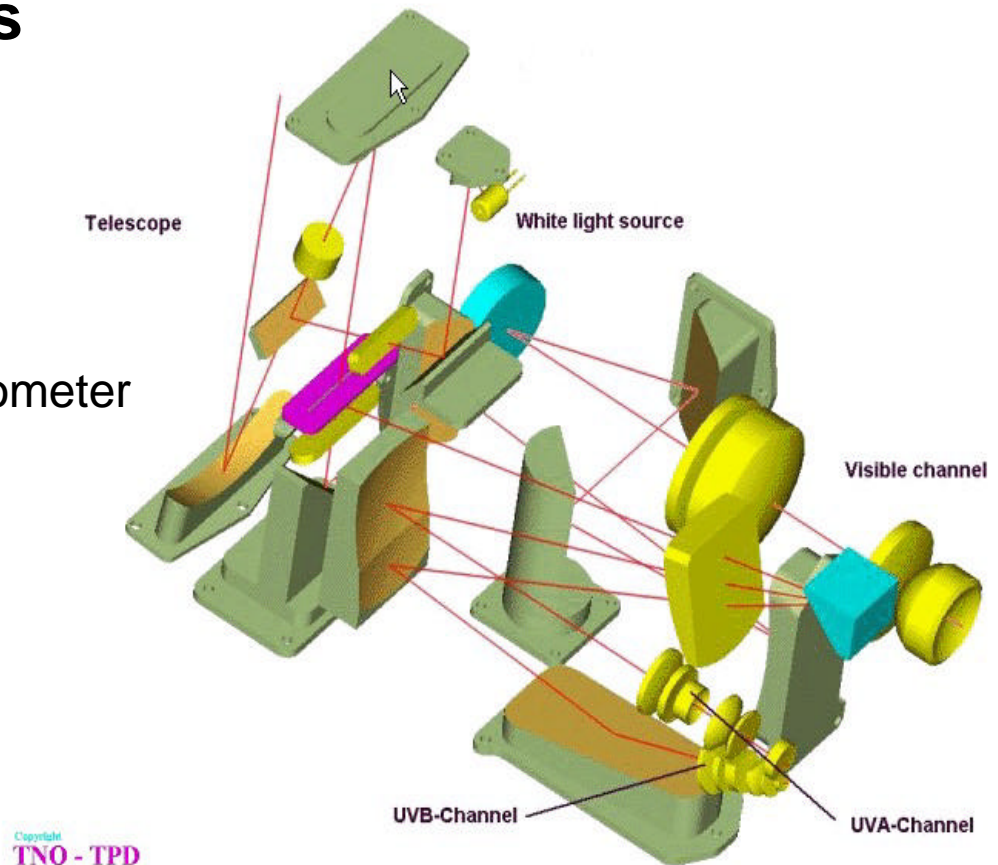
† H₂O is measured in the visible and infrared.

‡ Additional species are measured in the infrared.

Ozone Monitoring Instrument (OMI) - Aura

Instrument characteristics

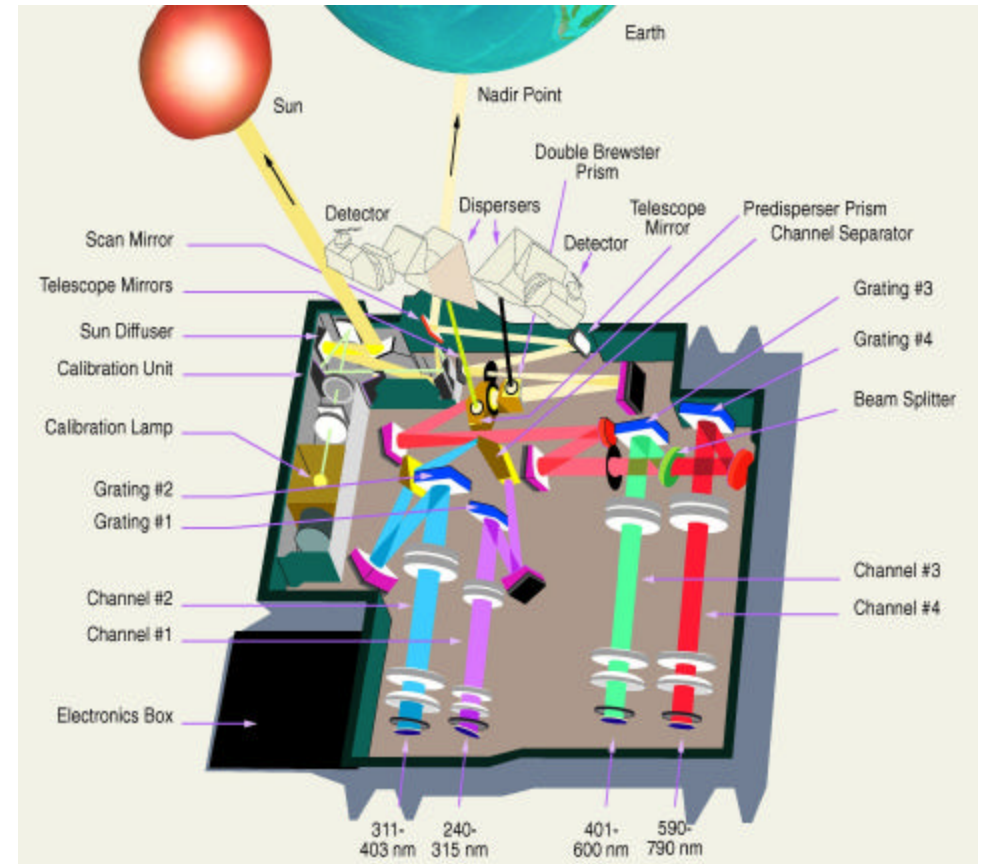
- 114 Telescope FOV (2600 km)
- 13X24 km IFOV
- Two channel hyperspectral spectrometer
UV: 270-380 nm
VIS: 350-500 nm
- 1.0 to 0.45 nm FWHM
- 2-3 samples per FWHM



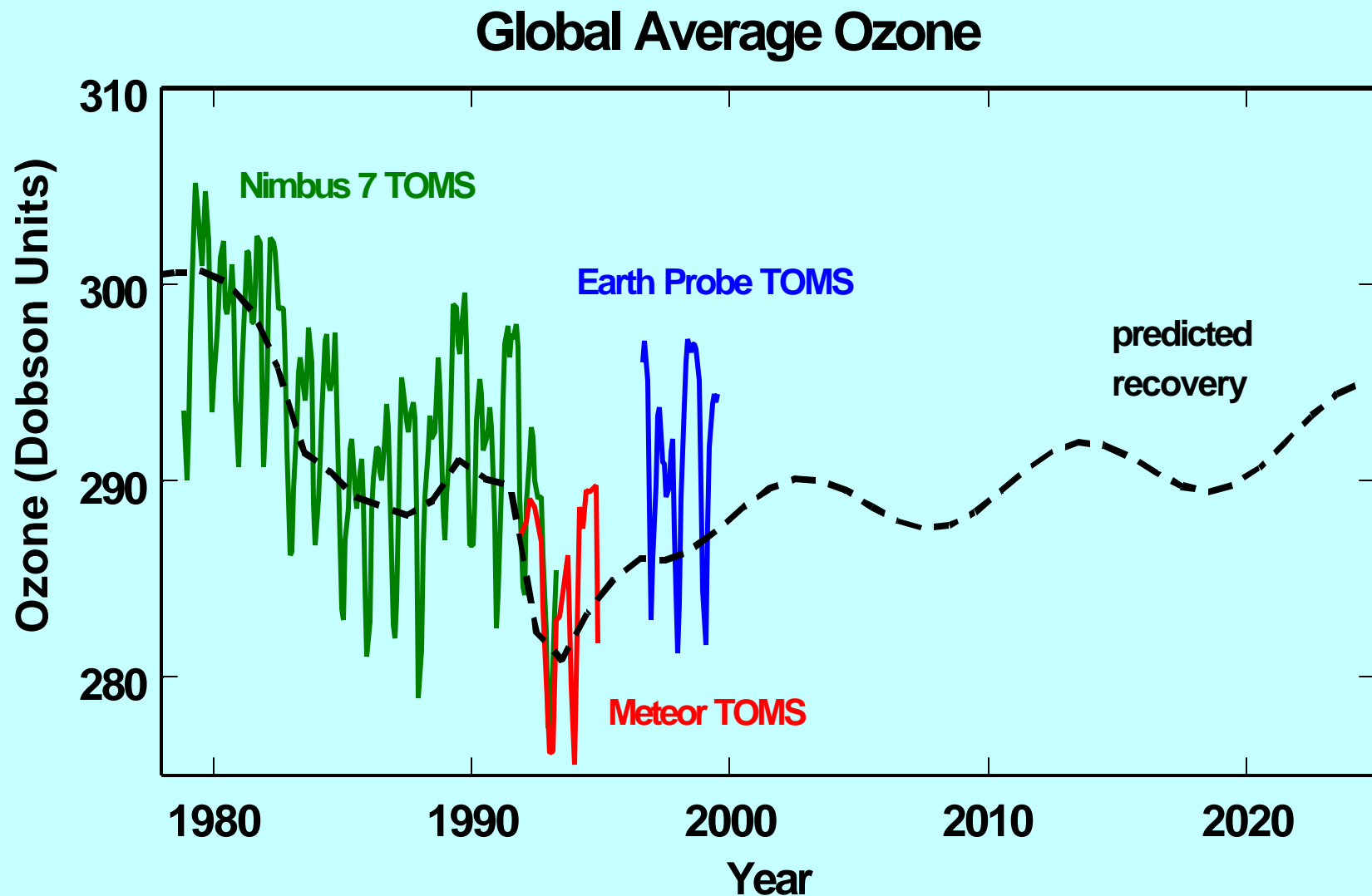
GOME-2 – Metop

Instrument characteristics

- Scan mirror swath is >960 km
- 40X80 km IFOV
- Four channel hyperspectral spectrometer
 - CH1: 240-315 nm
 - CH2: 309-403 nm
 - CH3: 401-600 nm
 - CH4: 590-790 nm
- 0.28 to 0.5 nm FWHM
- >2 Samples per FWHM

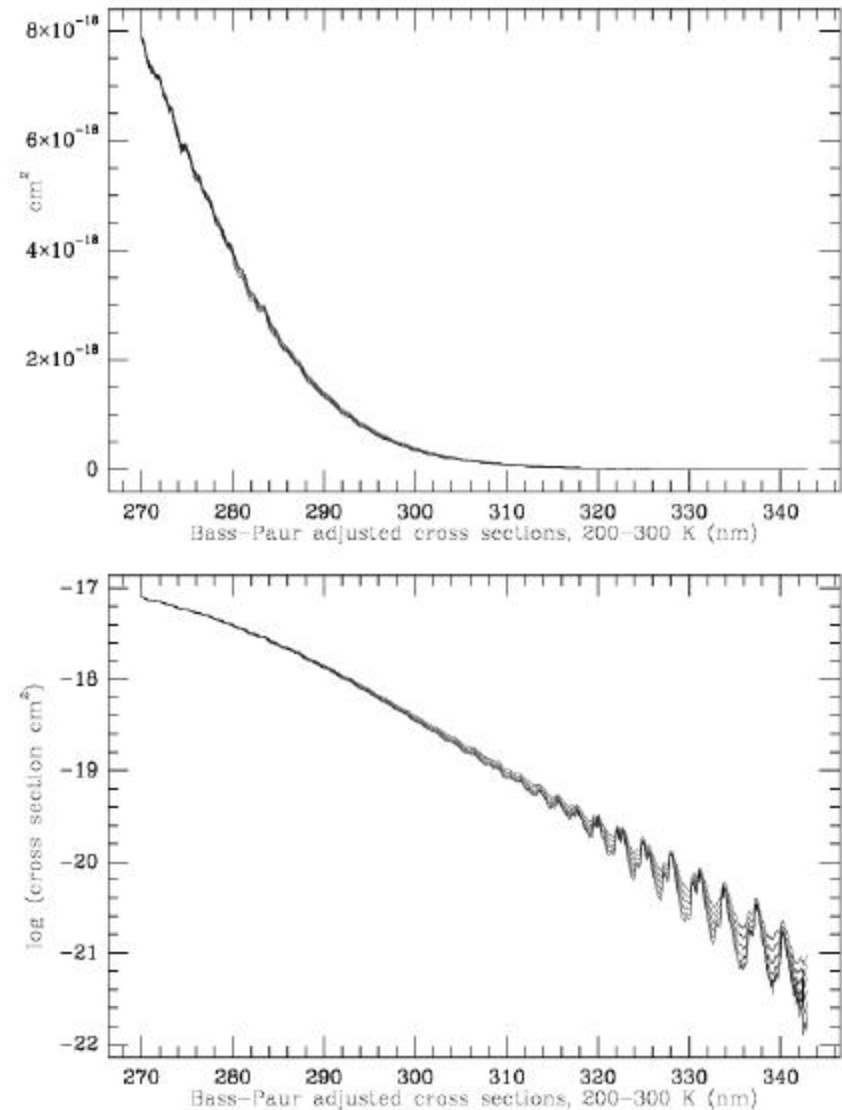


Detecting an ozone recovery requires a consistent observing system



O₃ Spectroscopy

- Agree with J. Orphal [2001] that B&P cross sections are acceptable and should be used by all space missions.
- Wavelength scale should be adjusted according to Edlén [1966], with an additional +0.015 nm shift.
- Bogumil et al. [2000] should be published (corrected to B&P) for wavelengths range 340-790 nm.
- Up to date measurements are planned in US (NIST) and France (NPM) using FTS:
 - 240-1000 nm @ 0.001 nm
 - 200° to 300°
 - <2% accuracy



NO₂ observed in stratosphere and troposphere

- NO₂ is important gas in stratospheric chemistry, air quality in troposphere.
- GOME instrument detects global seasonal variation and pollution hot spots.

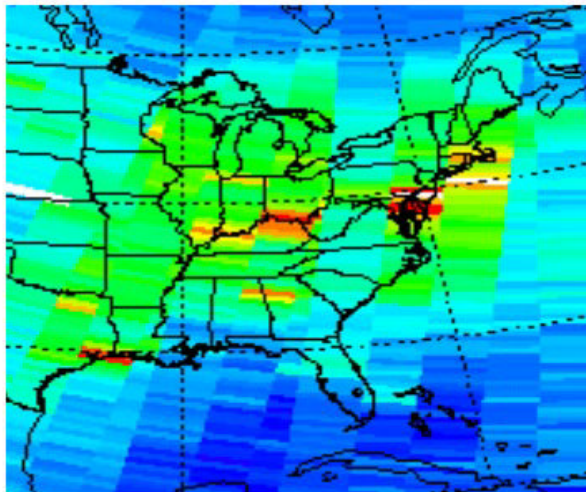
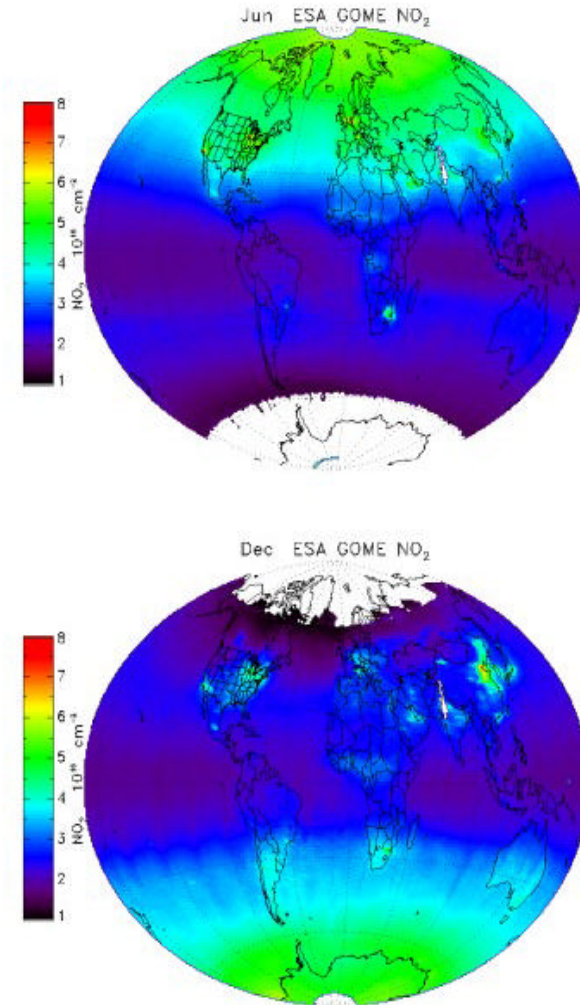
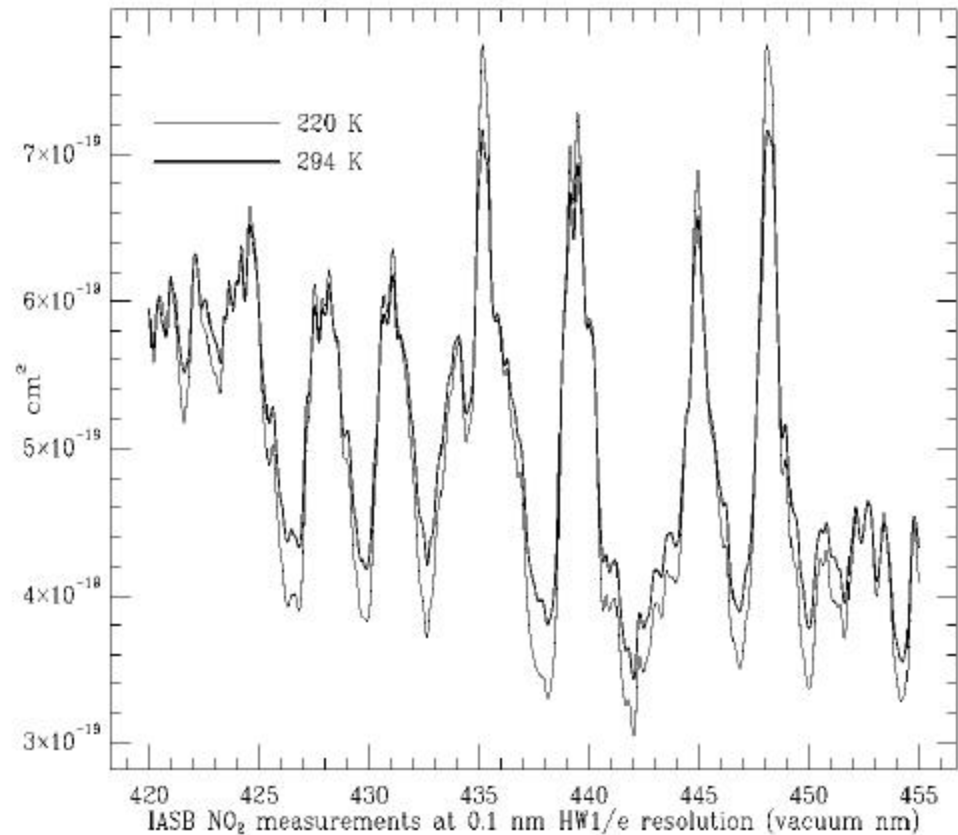


Figure 2.2 3-Day Composite of GOME NO₂ in April 1998. Scale as Figure 1.



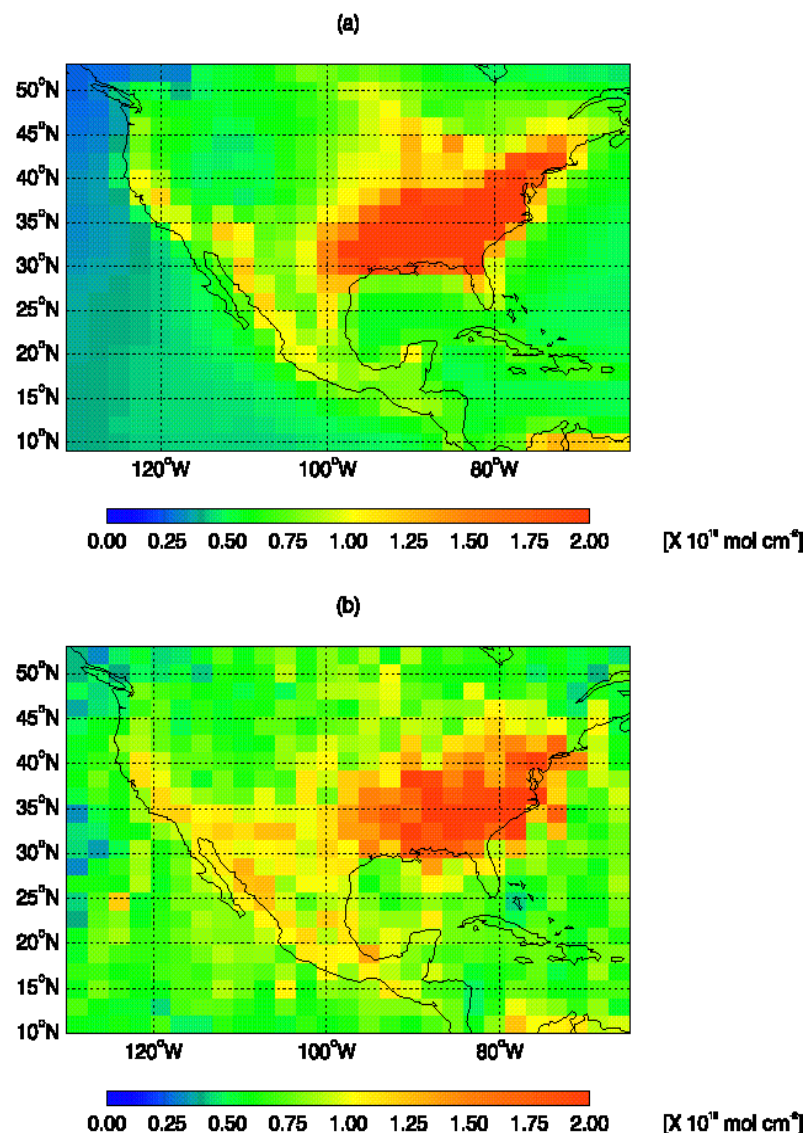
NO₂ Spectroscopy

- Vandaele et al. [1998] should be used as primary standard.
- Some uncertainty in wavelength calibration (0.0012 nm) because of air to vacuum conversion.
- 3% intensity uncertainty might be improved.
- Instrument builders opt to measure NO₂ with flight unit to test ITF (slit functions).



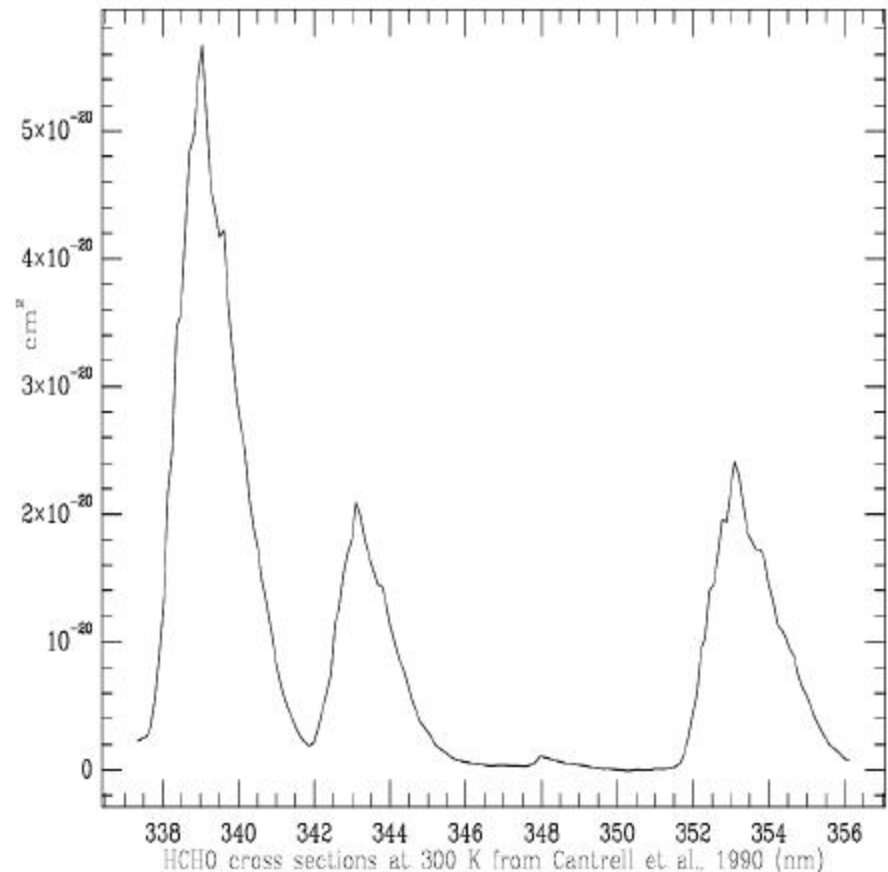
HCHO Observations from space

- HCHO is intermediate in oxidation of hydrocarbons in the troposphere, providing an important indicator of biogenic activity.
- Top, (a) Vertical column of HCHO from GOME measurements over North America for July 1996;
- Bottom, (b) Modeled result from the GEOS-CHEM 3-dimensional tropospheric chemistry and transport model (July, 1996).



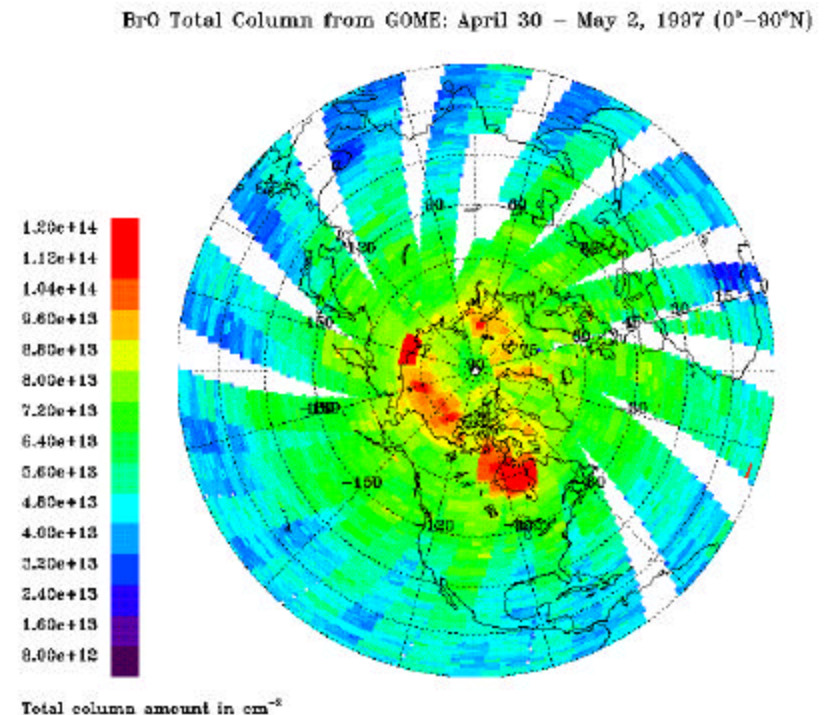
HCHO Spectroscopy

- Cantrell et al. [1999] are adequate for current space applications.
- 5% uncertainty with temperature dependence of 5% in troposphere.
- Uncertainties are negligible compared to other errors, e.g., air mass factors.



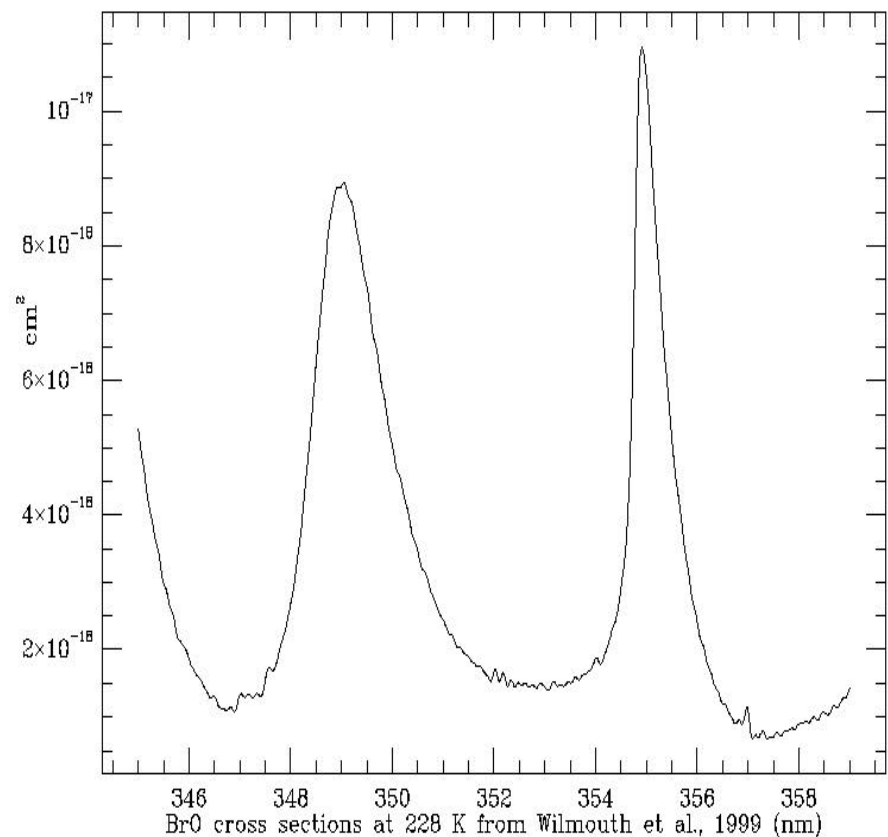
BrO observations from space

- BrO is a strong source of O_3 destruction in the stratosphere.
- BrO is measured globally by GOME.
- Enhanced tropospheric BrO has been observed over the Arctic and Antarctic ice pack in the polar spring.
- Quantifying tropospheric BrO from nadir (GOME, OMI) measurements is difficult due to the effect of Rayleigh scattering on air mass factors.



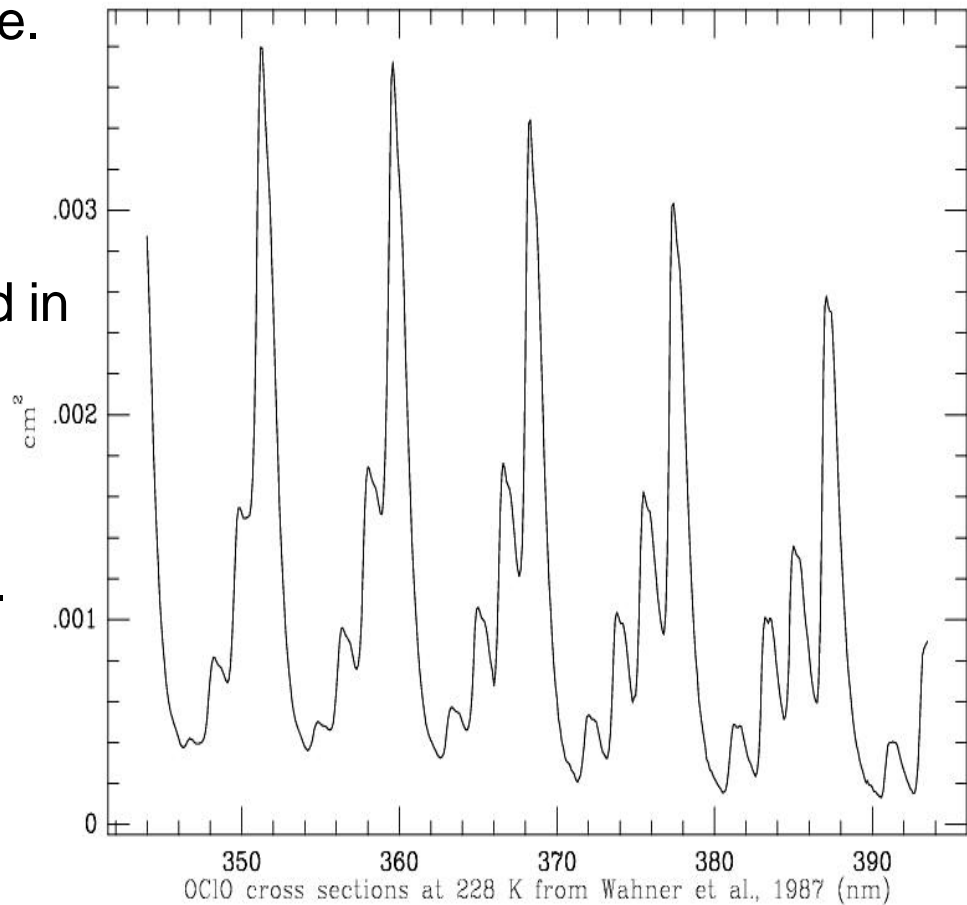
BrO Spectroscopy

- Wilmouth et al. [1999] are excellent for present applications.
- Measured at two temperatures. Uncertainty is negligible compared to other errors, e.g., air mass factors.



OCIO Spectroscopy

- Wahner et al. [1987] are adequate. Measured in air at three temperatures.
- Should eventually be re-measured in vacuum, with an FTS.
- Cross section errors are small compared to other retrieval errors.

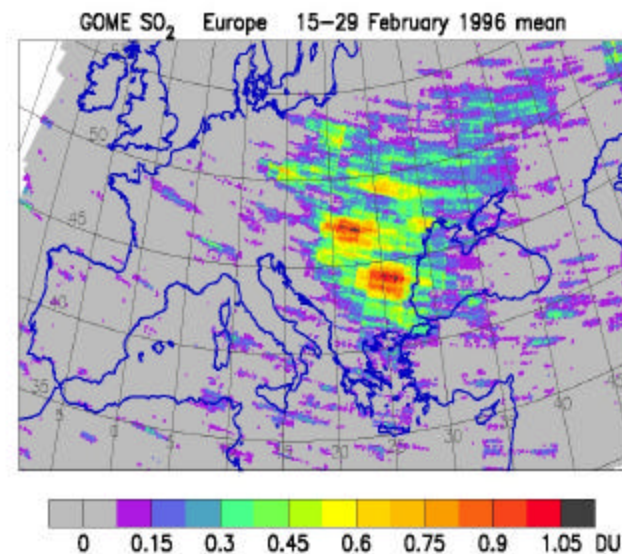
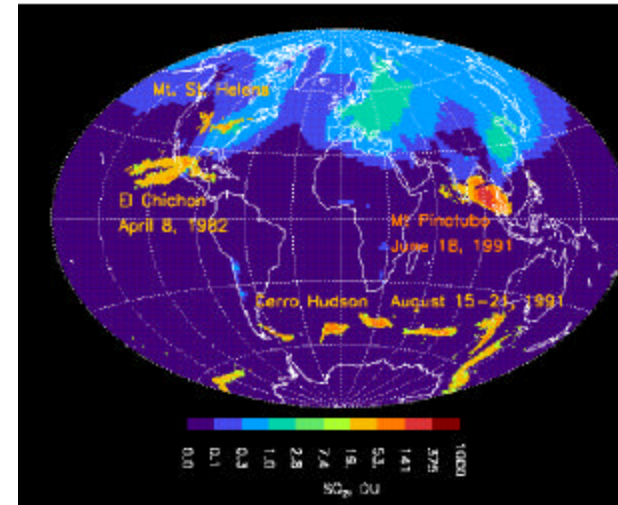


SO₂ observed in stratosphere and troposphere

TOMS has detected and mapped large Volcanic events since 1978 using wavelength channels designed for ozone. S/N not suitable for SO₂ tropospheric detection.

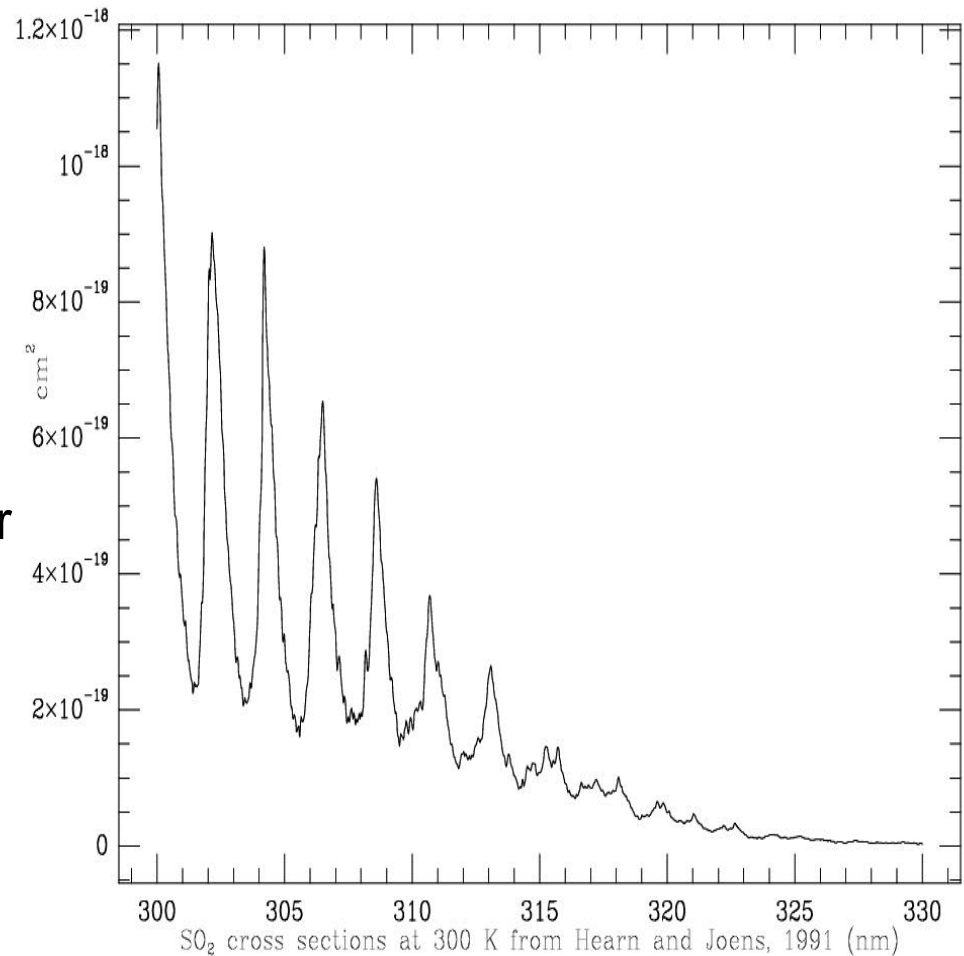
Spectral fitting (DOAS) techniques takes advantage of multiple wavelengths to improve S/N allowing tropospheric amounts to be retrieved.

OMI SO₂ algorithm will take advantage of spectral fitting with R/T model.



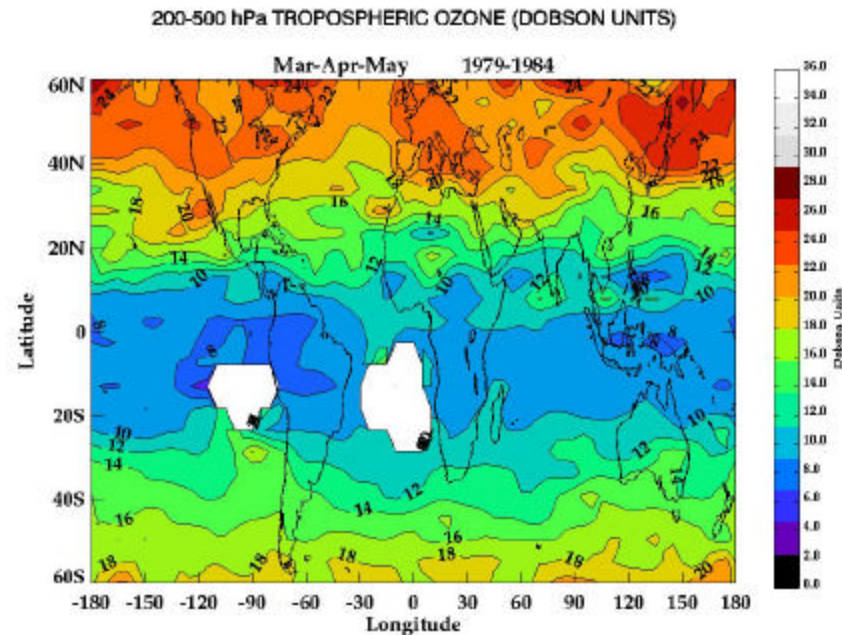
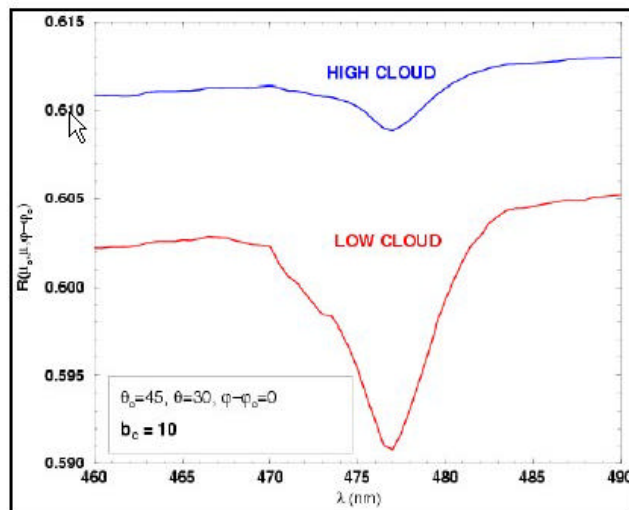
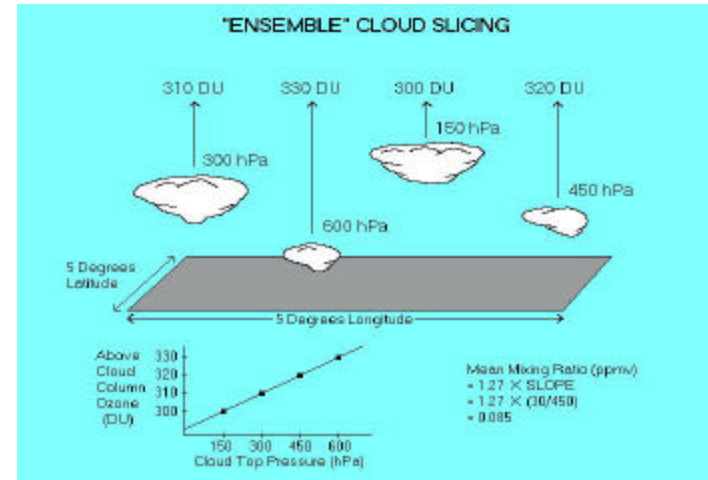
SO₂ Spectroscopy

- Hearn and Joens [1991] are barely adequate (300°).
- McGee and Burris [1987] have better resolution and measured at 295° and 210°.
- Measurements need to go to higher wavelengths, 327 nm, at multiple temperatures, to cover retrieval window.



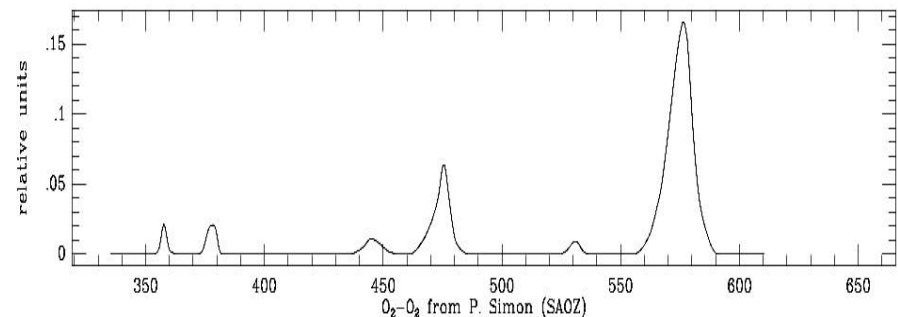
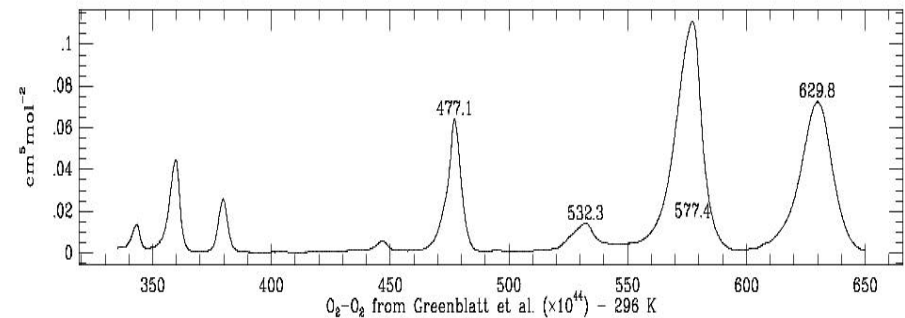
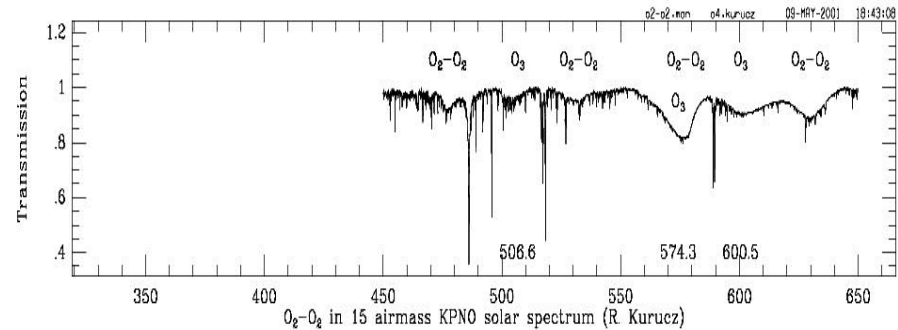
Cloud top heights from O_2-O_2

- Cloud top heights needed for accurate total ozone retrievals.
- Column density of O_2-O_2 is related to cloud top heights
- Cloud top heights can be used for tropospheric ozone profiles.



O₂-O₂ Spectroscopy

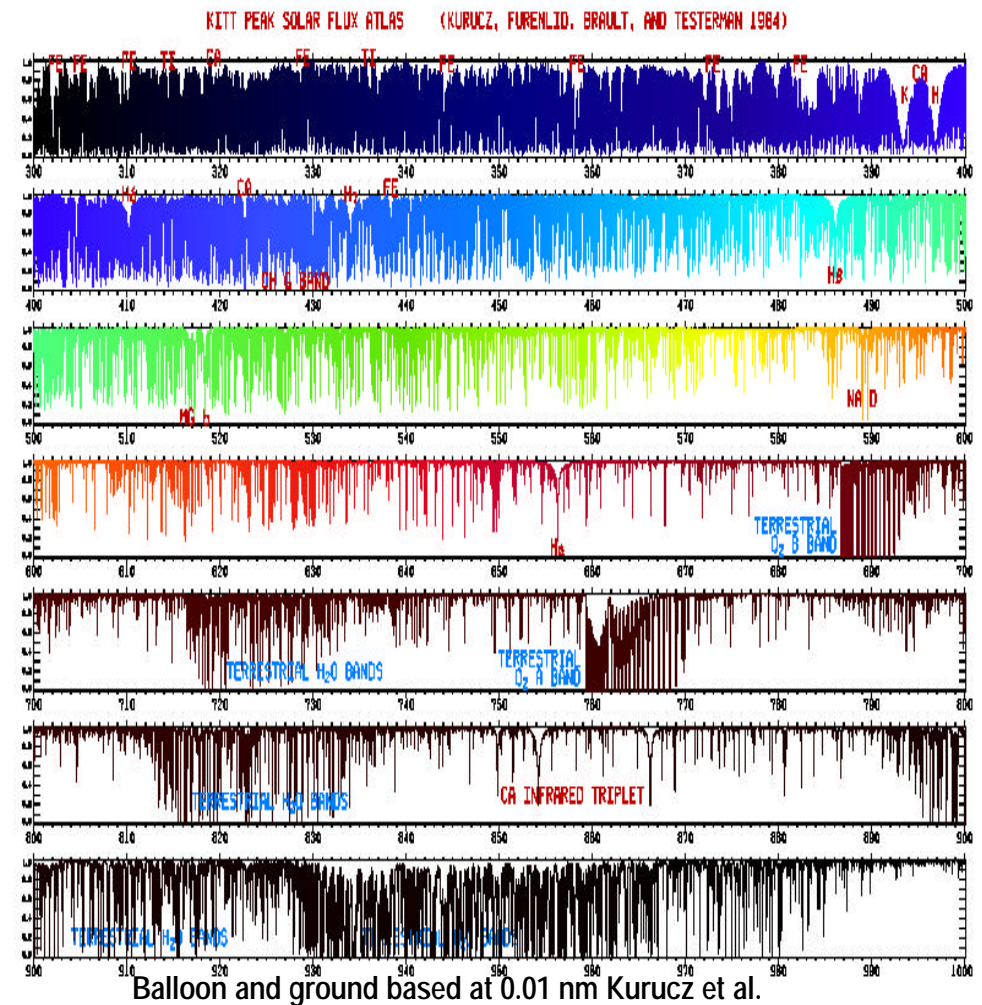
- Greenblatt et al., [1990] only data in UV/VIS. UV data needed for spectral fitting.
- Intensities are +/- 10%, not an issue for trace gas retrievals.
- Requires correction to vacuum and wavelength re-calibration.
- Need cross section vs. temperature, only available at 296°.
- Newman and Ballard [1998] with T, P dependence are best for cloud height detection. They do not extend to BrO, OCIO, HCHO fitting regions.



TOA Solar spectral irradiance

High resolution solar spectral irradiance would be very useful in analyzing atmospheric trace gases:

- Solar lines are source of accurate wavelength calibration.
- Better characterization of the Ring effect.
- Improved knowledge of instrument slit functions.
- Correction for spectral undersampling.
- Photochemistry of Schumann-Runge system.
- **Requirements:**
 - Range: 240-1000 nm
 - FWHM: 0.01 nm
 - Ideal FTS Space Shuttle experiment.



Summary

- Spectroscopy of gases observed in UV/VIS are in pretty good shape. Their uncertainty is not a significant contribution to measurement error.
- Some of these gases could use the same treatment given by Orphal [2001] in his review of O_3 and NO_2 .
- Measurements using standard techniques (e.g. FTS) are needed and should be applied to all space missions to insure consistent data sets.
- Spectroscopy of gases measurable by reflected radiation in NIR was not discussed but should be reviewed.
- Aerosols are being routinely observed in UV/VIS. Spectroscopy of various types needs further study (e.g. index of refraction).

Acknowledgements

Harvard University

R. Martin, P. Palmer, D. Jacob

Royal Dutch Meteorological Institute (KNMI)

J.R. Acarreta, J.F de Haan

CNRS/Université Paris-Sud

J. Orphal

Smithsonian Astrophysical Observatory

R. Kurucz, L. Rothman, T. Kurosu

University of Bremen/AWI

M. Eisinger, J. Burrows

University of Maryland

A. Krueger

NASA Goddard Space Flight Center

J. Gleason, S. Chandra, C. Jackman

Eumetsat

NIVR

NASA Headquarters